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Title: Actinides: What we should do and what we do--and how to connect the two

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Actinides: What we should do and what we do—and how to connect the two

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Materials and Physics data, XCP-5

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Dirac equation

orbitals to densitals

Dirac-based DFT

Orbital: Ψ_i not an observable

Electron density: $\sum_i f_i |\Psi_i|^2$ an observable

Probability density: $|\Psi_i|^2$

Densital: $|\Psi_i|^2 > \text{cutoff}$

Schrödinger equation

orbitals to densitals

SE-based DFT

Non-relativistic limit

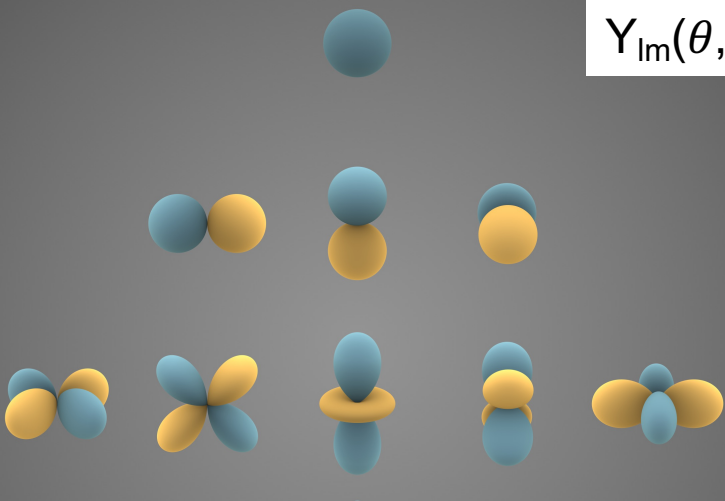
What we do



Orbitals

n, l, m, spin

$$Y_{lm}(\theta, \psi)$$



Densitals

N, j, j_3, κ

$$|g_{N\kappa} \mathcal{Y}_{j,j_3}(\theta, \psi)|^2$$

$$j_3 = \pm 5/2$$

$$\kappa < 0$$

$$j_3 = \pm 3/2$$

$$\kappa < 0$$

$$j_3 = \pm 1/2$$

$$\kappa < 0$$

$$j_3 = \pm 1/2$$

$$\kappa > 0$$

$$j_3 = \pm 3/2$$

$$\kappa > 0$$

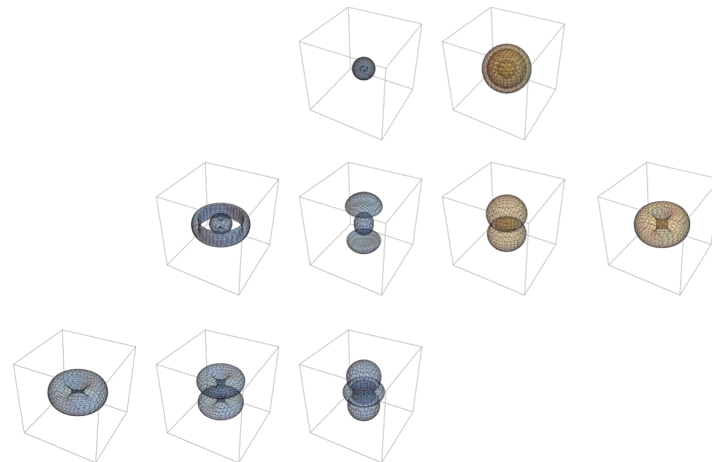
$$j_3 = \pm 5/2$$

$$\kappa > 0$$

$j = 1/2$

$j = 3/2$

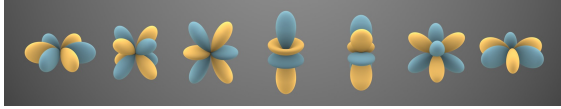
$j = 5/2$



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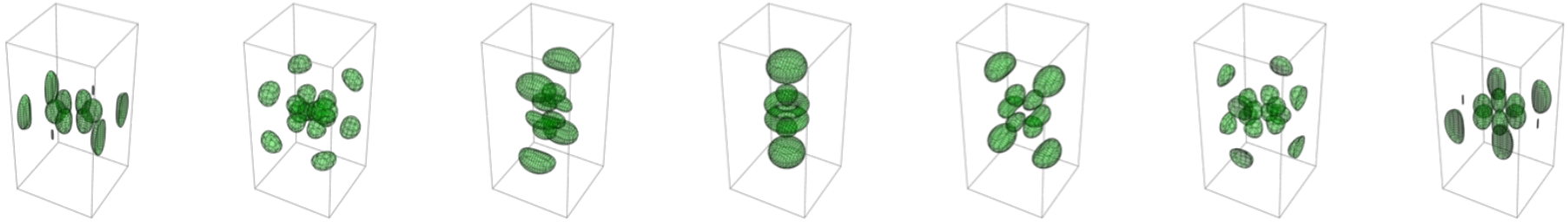
Hydrogen-like atom with non-interacting electrons



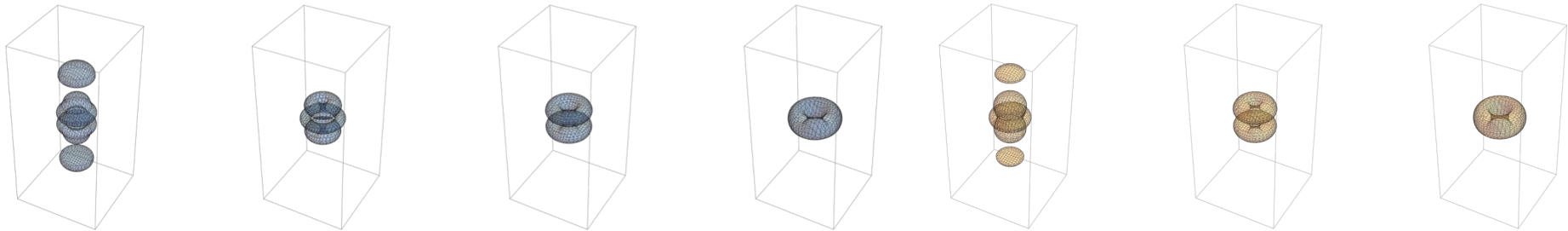
Schrödinger Equation

Real spherical harmonics

5f $m=-3,-2,-1,0,1,2,3$
Spin-up and spin-down
gives 14 electrons



Dirac Equation



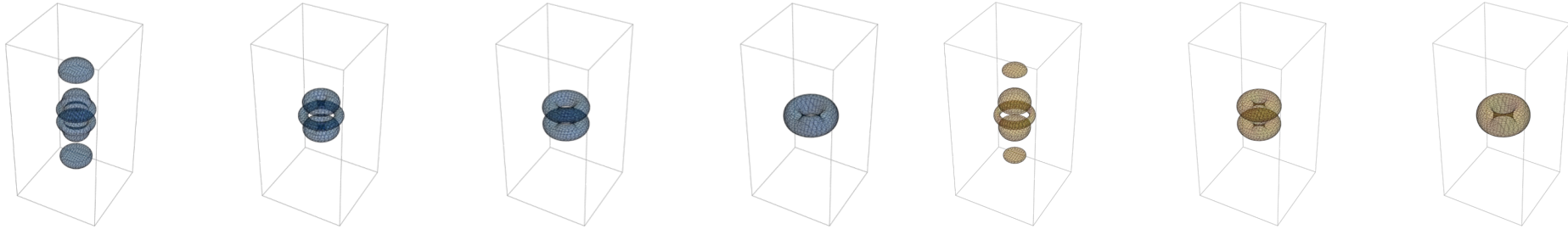
5D^hf (4 each of $\pm j_3$), 5D^f (3 each of $\pm j_3$) total 14 electrons



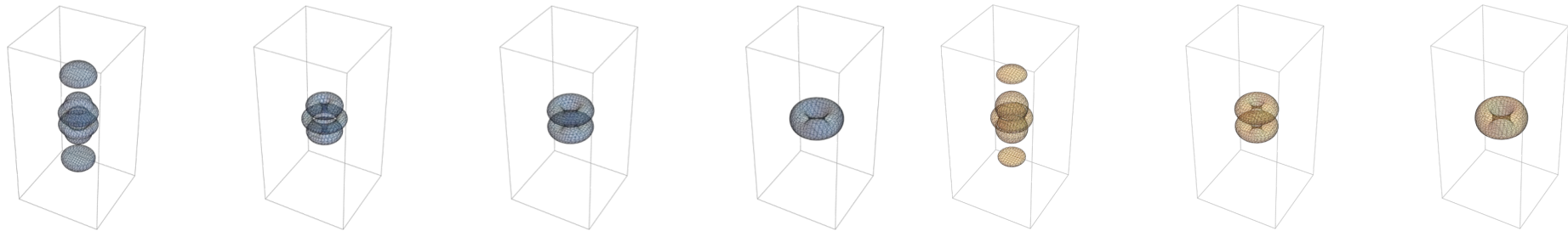
Hydrogen-like atom with non-interacting electrons

Dirac spherical harmonics

Schrödinger Equation



Dirac Equation



$5D^{hf}$ (4 each of $\pm j_3$), $5D^{lf}$ (3 each of $\pm j_3$) total 14 electrons



As no Dirac-DFT codes are available (yet) we need to interpret Schrödinger equation solutions from a Dirac equation viewpoint.

We can get densitals from the Schrödinger equation that correspond well to the Dirac densitals for the same problem.

Future work: Use the insights gained from this new viewpoint to revolutionize DFT based calculations for actinides.

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